Chapter 6

Conclusions and Future Work

6.1 Conclusions

This thesis presented the development of a new discrete element method (DEM) based on Non-Uniform Rational Basis Splines (NURBS). Through NURBS, the new DEM is able to capture sphericity and angularity, the two particle morphological measures used in characterizing real grain geometries.

By taking advantage of the parametric nature of NURBS, the Lipschitzian *di*viding *rect*angle (DIRECT) global optimization procedure is employed as a solution procedure to the closest-point projection problem, which enables the contact treatment of non-convex particles. Indeed, the implementation ease of the new DEM is largely attributed to the DIRECT algorithm.

A contact dynamics (CD) approach to our NURBS-based discrete method is also formulated. By combining particle shape flexibility, properties of implicit time integration (e.g., larger time steps), and non-penetrating constraints, as well as a reduction to a static formulation in the limit of an infinite time step, we target applications in which the classical DEM either performs poorly or simply fails, i.e., in granular systems composed of rigid or highly stiff angular particles and subjected to quasistatic or dynamic flow conditions. The CD implementation is made simple by adopting a variational framework, which enables the resulting discrete problem to be readily solved using off-the-shelf mathematical programming solvers.

We demonstrated the capabilities of our NURBS-based DEM through 2D numerical examples that highlight the effects of particle morphology on the macroscopic response of granular assemblies under quasistatic and dynamic flow conditions, and a 3D characterization of material response in the shear band of a real triaxial specimen. In the latter case, we performed the first quantitative comparison of microscopic quantities from discrete simulation and experiment, and we found excellent agreement between the global continuum response calculated from multiscale computation using the extracted microscopic quantities and that measured from experiment.

6.2 Future Work

Many possible directions can be taken in the future to further the scope of application of our NURBS-based DEM. An immediate step would be the 3D CD implementation, which will enable a robust treatment of quasistatic loading conditions typically encountered in real triaxial experiments. The computational expense in our current implementation prohibits large calculations. Further algorithmic improvements, as well as a parallel computational scheme, are necessary to move forward with larger calculations and obtain more realizations for homogenization. We note that the unit cells considered in the 3D application are only an idealization of the actual system in terms of the boundary conditions, and we have made simplifying modeling assumptions to make the simulations tractable. The ability to perform a full specimen-level calculation would remedy this and provide us with quantities such as the complete stress state inside the shear band, which is currently inaccessible by experiment. A full specimen-level calculation will also allow one to look into the effects of specimen heterogeneity on the conditions for the development and propagation of shear bands, a study that is incomplete with only unit cell calculations. Finally, an improved computational scheme would allow us to study specimens composed of more angular grain geometries (e.g., Hostun sand).

From the 3D application described in the previous chapter, it is clear that our NURBS-based DEM has a great potential for complementing experimental problems related to the characterization of granular micromechanical properties. Currently, we have used data from only one triaxial experiment, which is severely limited. To make the characterization process more comprehensive, more experiments should be performed to probe how specific microscopic quantities or plastic internal variables may respond under different conditions (e.g., confinement pressure), and these would provide further validation cases for our method. Physical grain-scale experiments such as compression tests for contact response and scratch tests for interparticle friction can also be carried out. In general, both macro- and grain-scale experiments would serve to provide tighter bounds or constraints on the discrete model parameters.

We close this thesis by asking the following (hard) questions concerning the representation of particle geometry for grain-scale analysis, in which the answers are currently unclear and may become important when more angular geometries are considered:

1. How much geometric resolution does one need for grain-scale DEM to be accurate?
2. How sensitive is the macroscopic response to the level of geometric resolution?
3. Is there a scale separation between roundness and surface roughness? If not, how does one decide the spatial resolution cutoff below which the asperities are accounted for by interparticle friction.

Here, ideas from signal processing and statistical methods may provide quantitative means to start addressing these questions.